

**METADATA AND NUMERICAL DATA CAPTURE:
Viscosity
(2 – Components)**

***Guided Data*
Capture (GDC)**



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Viscosity**
(2-components)
with the **Guided Data Capture (GDC)** software.

NOTE:

The tutorials proceed sequentially to ease the descriptions. **It is not necessary to enter *all* compounds before entering *all* samples, etc.**

Compounds, samples, properties, etc., can be added or modified at any time.

However, the hierarchy must be maintained (i.e., a property cannot be entered, if there is no associated sample or compound.)

The experimental data used in this example is from:

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J. Chem. Eng. Data 2002, 47, 216–218

Densities, Viscosities, and Surface Tensions of the Trifluoroethanol + Quinoline System

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Densities, viscosities, and surface tensions of 2,2,2-trifluoroethanol (TFE) + quinoline were measured at various temperatures and concentrations. This system was chosen as it is a possible candidate for an organic working pair for an absorption heat pump. All results were correlated by a polynomial equation as a function of temperature and concentration, and the parameters of the regression equation were determined by a least-squares method. The average absolute deviations between the experimental and calculated values in the density, viscosity, and surface tension measurements were 0.12, 1.8, and 0.76%, respectively. The density values decreased with increasing temperature and quinoline mass fraction. As the temperature of the liquid mixture increased and the quinoline mass fraction decreased, the viscosity and surface tension values decreased.

**Viscosities (η) for the binary system
2,2,2-trifluoroethanol + quinoline
at $p = 101.3$ kPa and various temperatures**

**Table 2. Measured Viscosities (η) for the
2,2,2-Trifluoroethanol (1 - w) + Quinoline (w) Mixtures**

w	$\eta/\text{mPa}\cdot\text{s}$ at the following T/K					
	298.15	303.15	308.15	313.15	318.15	323.15
0.00	1.73	1.53	1.35	1.21	1.09	0.98
0.20	2.34	2.05	1.84	1.62	1.46	1.32
0.40	2.91	2.57	2.27	2.04	1.83	1.65
0.60	3.14	2.79	2.46	2.21	2.00	1.82
0.80	3.17	2.80	2.49	2.25	2.05	1.87
1.00	3.36	3.01	2.68	2.43	2.21	2.03

**This data set is
considered here.**

Experimental Method Info:

(ii) Viscosity Measurement. The viscosities of the binary mixture were measured with three appropriate Ubbelohde viscometers. The equipment and procedure used for the viscosity measurement were the same as those for our previous investigation.^{7,9} A suitable viscometer was selected considering the viscosity values. The viscometer was put into a bath whose temperature was controlled with a bath circulator within ± 0.05 K. The equilibrium time was about 15 min. The efflux time of the liquid solution through the capillary was measured manually with a stopwatch.

The dynamic viscosity values were calculated from

$$\eta = Kt\rho \quad (1)$$

where η is the dynamic viscosity, K the instrument constant, t the efflux time, and ρ the density of the sample.

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Reaction **Property** Data Tables

- 2002 kim lee 0
 - 2,2,2-trifluoroethanol
 - Sample 1 (cm,99x%,nc,;)
 - quinoline
 - Sample 1 (cm,99x%,nc,;)
 - 2,2,2-trifluoroethanol + quinoline**

2. CLICK
Property

1. SELECT the *mixture* for which the data are to be captured.

NOTE: The **bibliographic information, compound identities, sample descriptions, and mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)

Property and experimental method for 2,2,2-trifluoroethanol + quinoline

Help

Property group: Transport properties

Property: Viscosity

Units: mPa*s

Method of measurement:

Experimental purpose:

OK Cancel

1. SELECT the **Property Group:** *Transport properties* from the menu.

2. SELECT the **Property:** *Viscosity* for this example.

3. SELECT the **Units:** mPa*s, here. **SELECT ALL OTHER UNITS** if another multiplier is needed.

1. SELECT Method of Measurement from the list provided. **NOTE:** *Other* can be a valid selection and should include a brief description in the **Comment** field.

Units: mPa*s

Method of measurement: Capillary tube (Ostwald; Ubbelohde) method

Experimental purpose: Principal objective of the work

Comment (optional)

3. CLICK OK

OK Cancel

2. SELECT the Experimental Purpose from the list provided.

SELECTION of # of Phases in Equilibrium and # of Constraints

Viscosity (mPa*s) as function of 2 variable(s)

Mixture: 2,2,2-trifluoroethanol + quinoline

Phases in equilibrium: 1

Constraints: 1

Independent variables: 2

Phase of the Property Value(s)

SELECT the # of **Phases in equilibrium**. There is **1** phase; *liquid*.

SELECT the # of **Constraints**. There is **1** constraint in the present example; *pressure*.

Viscosity (mPa*s) as function of 2 variable(s)

Mixture: 2,2,2-trifluoroethanol + quinoline

Phases in equilibrium: 1 Constraints: 1 Independent variables: 2 Property set #: 1

Sample #: 1 Sample #: 1

Phase of the Property Value(s):

Definition of Measurement Results (Absolute vs Relative):

Data presentation: Experimental values

Solvent:

Comments (Optional):

Property and method Numerical Data Cancel

Multiple *samples* for a given component can be accommodated, but this is rarely needed.

Viscosity (mPa*s) as function of 2 variable(s)

Mixture: 2,2,2-trifluoroethanol + quinoline

Phases in equilibrium: 1 Constraints: 1 Independent variables: 2 Property set # 1 Sample # 1 Sample # 1

Phase of the Property Value(s) Liquid

Constraint 1 (Fixed value of) Liquid

Independent variable 1 Liquid

Independent variable 2 Liquid

1) SELECT *Liquid* from the list provided for the **Phase of the Property Value**

NOTE: Constraint and Independent Variable field(s) appear automatically based on the Gibbs Phase Rule.

Specification of constraints, constraint values, and constraint units

1. SELECT the **Constraint(s)** (p here) and the **Independent Variable(s)** (T and w_1 , here) from the lists provided.

Mixture: 2,2,2-trifluoroethanol + quinoline
Phases in equilibrium: 1 Constraints: 1 Independent variables: 2 Property set # 1 Sample # 1 Sample # 1
Phase of the Property Value(s) Liquid Precision of the Property Value(s) mPa*s

Constraint 1 (Fixed value of)
Pressure of Liquid Value: 101.3 Units: kPa Uncertainty: %

Independent variable 1
Temperature of Liquid Units: K Uncertainty: 0.05 %

Independent variable 2
Weight fraction of 2,2,2-trifluoroethanol of Liquid Units: Dimensionless Uncertainty: %

Definition of Measurement Results (Absolute vs Relative)

Data presentation

Experim

Com

2. TYPE the Constraint **Value(s)** (101.3 , here) and SELECT **Units** for the Variable(s) and Constraint(s). Include **Uncertainties**, if known.

Measurement definition and Data presentation

Viscosity (mPa*s) as function of 2 variable(s)

Mixture: 2,2,2-trifluoroethanol + quinoline

Phases in equilibrium: 1 Constraints: 1 Independent variable

Phase of the Property Value(s) Liquid

Constraint 1 (Fixed value of) Pressure of Liquid

Independent variable 1 Temperature of Liquid

Independent variable 2 Weight fraction of 2,2,2-trifluoroethanol of Liquid

Units: Dimensionless Uncertainty: 0.05 %

Definition of Measurement Results (Absolute vs Relative)
Direct value

Data presentation
Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

1. SELECT *Direct Value* (as compared with *Relative Value*) from the list defining the **Measurement Results**

2. SELECT the appropriate **Data presentation** method. *Experimental values* here.

3. CLICK *Numerical Data*

Viscosity (mPa*s) as function of 2 variable(s)

File Edit Action Help

	Var 1	Var 2	Property
1			

TYPE, or much preferably, PASTE the variable and property values into the table. See next page...

Table 2. Measured Viscosities (η) for the 2,2,2-Trifluoroethanol (1 - w) + Quinoline (w) Mixtures

η /mPa*s at the following T/K

w	298.15	303.15	308.15	313.15	318.15	323.15
0.00	1.73	1.53	1.35	1.21	1.09	0.98
0.20	2.34	2.05	1.84	1.62	1.46	1.32
0.40	2.91	2.57	2.27	2.04	1.83	1.65
0.60	3.14	2.79	2.46	2.21	2.00	1.82
0.80	3.17	2.80	2.49	2.25	2.05	1.87
1.00	3.36	3.01	2.68	2.43	2.21	2.03

Clear the Table View plot Accept Cancel

Viscosity (mPa*s) as function of 2 variable(s)

File Edit Action Help

	Var 1	Var 2	Property
1	298.15	0.00	1.73
2	298.15	0.20	2.34
3	298.15	0.40	2.91
4	298.15	0.60	3.14
5	298.15	0.80	3.17
6	298.15	1.00	3.36
7	303.15	0.00	1.53
8	303.15	0.20	2.05
9	303.15	0.40	2.57
10	303.15	0.60	2.79
11	303.15	0.80	2.80
12	303.15	1.00	3.01
13	308.15	0.00	1.35
14	308.15	0.20	1.84
15	308.15	0.40	2.27
16	308.15	0.60	2.46
17	308.15	0.80	2.49
18	308.15	1.00	2.68
19	313.15	0.00	1.21
20	313.15	0.20	1.62
21	313.15	0.40	2.04
22	313.15	0.60	2.21
23	313.15	0.80	2.25
24	313.15	1.00	2.43
25	318.15	0.00	1.09

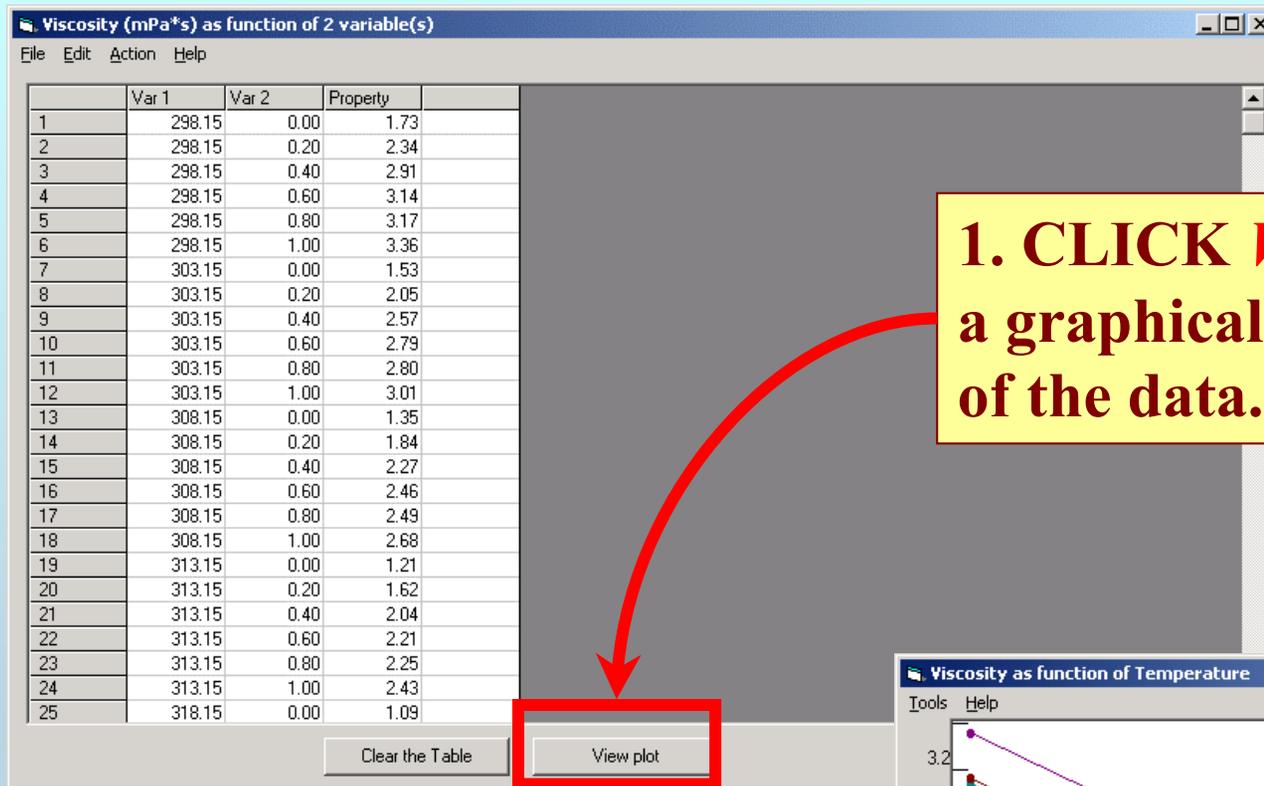
Clear the Table View plot Accept Cancel

Table 2. Measured Viscosities (η) for the 2,2,2-Trifluoroethanol (1 - w) + Quinoline (w) Mixtures

η /mPa*s at the following T/K

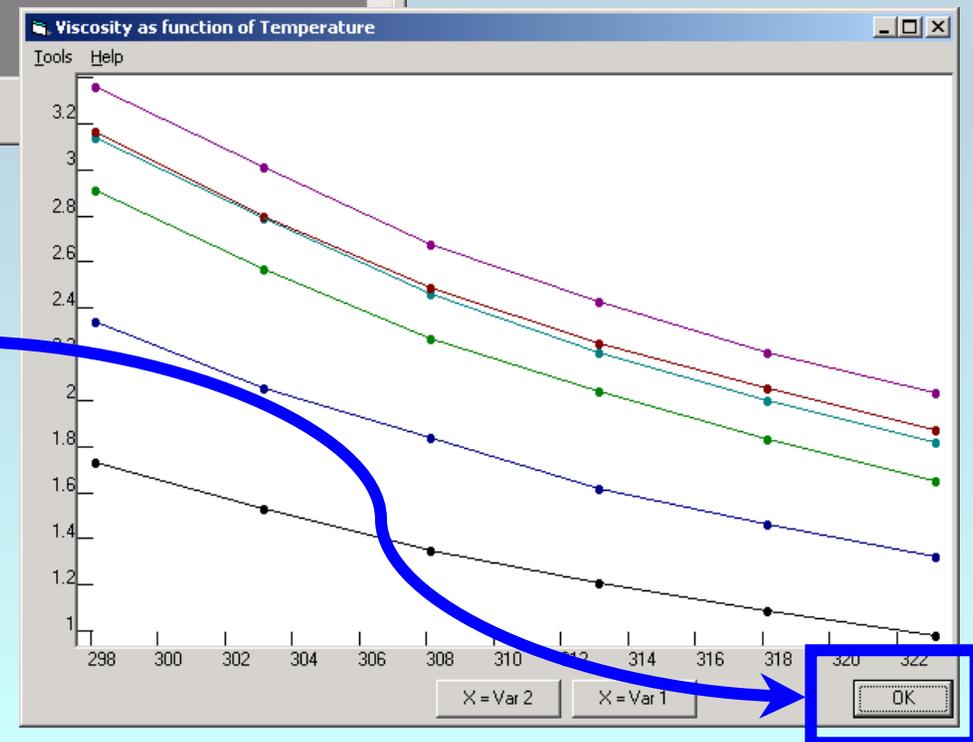
w	298.15	303.15	308.15	313.15	318.15	323.15
0.00	1.73	1.53	1.35	1.21	1.09	0.98
0.20	2.34	2.05	1.84	1.62	1.46	1.32
0.40	2.91	2.57	2.27	2.04	1.83	1.65
0.60	3.14	2.79	2.46	2.21	2.00	1.82
0.80	3.17	2.80	2.49	2.25	2.05	1.87
1.00	3.36	3.01	2.68	2.43	2.21	2.03

NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software, e.g., EXCEL.)



1. CLICK *View plot* to see a graphical representation of the data.

2. Check for typographical errors, and CLICK *OK*, when done.



Viscosity (mPa*s) as function of 2 variable(s)

File Edit Action Help

	Var 1	Var 2	Property
1	298.15	0.00	1.73
2	298.15	0.20	2.34
3	298.15	0.40	2.91
4	298.15	0.60	3.14
5	298.15	0.80	3.17
6	298.15	1.00	3.36
7	303.15	0.00	1.53
8	303.15	0.20	2.05
9	303.15	0.40	2.57
10	303.15	0.60	2.79
11	303.15	0.80	2.80
12	303.15	1.00	3.01
13	308.15	0.00	1.35
14	308.15	0.20	1.84
15	308.15	0.40	2.27
16	308.15	0.60	2.46
17	308.15	0.80	2.49
18	308.15	1.00	2.68
19	313.15	0.00	1.21
20	313.15	0.20	1.62
21	313.15	0.40	2.04
22	313.15	0.60	2.21
23	313.15	0.80	2.25
24	313.15	1.00	2.43
25	318.15	0.00	1.09

CLICK *Accept*

Clear the Table View plot **Accept** Cancel

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference

Compound

[-] 2002 kim lee 0

[-] 2,2,2-trifluoroethanol

... Sample 1 (cm,99x%,nc:)

[-] quinoline

... Sample 1 (cm,98x%,nc:)

[-] 2,2,2-trifluoroethanol + quinoline

... ^2: IST (Set 1), B Method:OTHER dIST=0.01 dT=0.05

... ^2: NVC (Set 1), B Method:CAPTUB dT=0.05

NOTE: The new data set now appears in the tree under the appropriate *mixture*.

NOTE: DOUBLE CLICKING on the *data set* allows editing of all entered information.

END

**Continue with other compounds,
samples, properties, reactions, etc...**

or save your file and exit the program.